

META-MODELS FOR PREDICTING BLOOD BRAIN BARRIER PENETRATION BASED ON SIMPLE PHYSICOCHEMICAL DESCRIPTORS

ABSTRACT OF THE INVENTION

5 Descriptor based models, employing at least two descriptors, predict activities
of compounds under consideration. Those activities may be biology-based activities
such as the ability of the compound to cross the blood brain barrier. In one example,
the model predicts a compound's solubility, its ability to be absorbed in the intestine,
and its ability to cross the blood brain barrier. The descriptors of interest are typically
10 physicochemical properties of the whole molecule. Examples include a log P or log D,
molecular weight or related size-based descriptors, the number of hydrogen bond
donors and/or hydrogen bond acceptors, formal charge, lipophilicity, and the like.